1

$1,2$

R

T

$reso(resampled)/reso(input)$

$t \times f_{\mathrm{res}} / T_{\mathrm{sys}}^2$

t

f_{res}

$1/\sigma^2$

σ

S

$(N-1)^{th}$

N^{th}

r_R

r_T

$$r_S = \max(|r_R|, |r_T|)$$

$x_{\min,S}$

$\min(x_{\min,R}, x_{\min,T})$

$\max(x_{\max,R}, x_{\max,T})$

$\max(x_{\min,R}, x_{\min,T})$

$\min(x_{\max,R}, x_{\max,T})$

N

$$N_S = \mathrm{int}(\frac{x_{\max,S} - x_{\min,S}}{r_S} + 1.5),$$

$$x_{\mathrm{val},S} = x_{\mathrm{min},S} - 1. \times r_S,$$

$x_{\min,S}$

x

$$\left[x_{\min,S}, x_{\max,S}\right]$$

N_S

$T(i)$

$w(i)$

Averaged channel intensity and weight (aligned spectra):

$$T_S(i) = \frac{w_R(i) \times T_R(i) + w_T(i) \times T_T(i)}{w_R(i) + w_T(i)} \quad (1)$$

$$w_S(i) = w_R(i) + w_T(i) \quad (2)$$

R'

T'

$k_{\min}$

T_R

i

$N(\mu_R, {\sigma_R}^2)$

$$\mathrm{pdf}_R(x) = \frac{1}{\sigma_R \sqrt{2\pi}} \exp\left(-\frac{(x-\mu_R)^2}{2{\sigma_R}^2}\right)$$

μ_R

σ_R

$$\mathrm{var}(T_R(i)) = \sigma_R(i)^2$$

$w_R(i)$

$$w_R(i) = \frac{1}{\sigma_R(i)^2}$$

Resampled channel intensity (all weights):

$$T_{R'}(i) = \frac{\sum_{j=j_{\min}}^{j_{\max}} f_R(j) \times w_R(j) \times T_R(j)}{\sum_{j=j_{\min}}^{j_{\max}} f_R(j) \times w_R(j)} \tag{3}$$

$$f(j) = 0$$

$$f(j) = 1$$

$0 < f(j) < 1$

$$\beta = \sum_{j=j_{\min}}^{j_{\max}} f_R(j) \times w_R(j)$$

$$\alpha_R(j) = \frac{f_R(j) \times w_R(j)}{\beta}$$

$$T_{R'}(i) = \sum_{j=j_{\min}}^{j_{\max}} \alpha_R(j) \times T_R(j)$$

$\mathrm{var}(T_{R'}(i))$

$$\mathrm{var}\left(\sum_{j=j_{\min}}^{j_{\max}} \alpha_R(j) \times T_R(j)\right)$$

$$\sum_{j=j_{\min}}^{j_{\max}} \alpha_R(j)^2 \times \operatorname{var}\left(T_R(j)\right)$$

$$\frac{1}{\beta^2} \sum_{j=j_{\min}}^{j_{\max}} f_R(j)^2 \, w_R(j)$$

$$\mathrm{var}(aX + bY) = a^2\mathrm{var}(X) + b^2\mathrm{var}(Y)$$

a

b

X

Y

Resampled channel weight (weights `TIME` and SIGMA):

$$w_{R'}(i) = \frac{\left(\sum_{j=j_{\min}}^{j_{\max}} f_R(j) w_R(j)\right)^2}{\sum_{j=j_{\min}}^{j_{\max}} f_R(j)^2 \, w_R(j)} \tag{4}$$

R'

0.25

$w_{R'}$

$\sigma_{R'}$

$x_{\mathrm{val}} \to x_{\mathrm{val}} + 0.00$

$$w_{R'} = w_R$$

$\sigma_{R'} = \sigma_R$

$x_{\mathrm{val}} \rightarrow x_{\mathrm{val}} + 0.25$

$$w_{R'} = 1.6 \times w_R$$

$$\sigma_{R'} = \sigma_R / \sqrt{1.6}$$

$x_{\mathrm{val}} \to x_{\mathrm{val}} + 0.50$

$$w_{R'} = 2 \times w_R$$

$$\sigma_{R'} = \sigma_R / \sqrt{2}$$

$\sqrt{2}$

$R' \to R''$

Resampled channel weight (weight `EQUAL`):

$$w_{R'}(i) = \frac{\sum_{j=j_{\min}}^{j_{\max}} f_R(j) w_R(j)}{\sum_{j=j_{\min}}^{j_{\max}} f_R(j)} \tag{5}$$

1.0

T_S

w_S

Averaged channel intensity and weight (non-aligned spectra):

$$T_S(i) = \frac{w_{R'}(i) \times T_{R'}(i) + w_{T'}(i) \times T_{T'}(i)}{w_{R'}(i) + w_{T'}(i)} \quad (6)$$

$$w_S(i) = w_{R'}(i) + w_{T'}(i) \quad (7)$$

$f \neq 0$

"

$$t_{S_{\text{out}}} = t_{S_{\text{in}}} + t_{\text{obs}}$$

$$T_{\mathrm{sys},S_{\mathrm{out}}}$$

$t \times |r|/T_{\mathrm{sys}}^2$

γ

$$\frac{t_{S_{\text{out}}} \times |r_{S_{\text{out}}}|}{T^2_{\text{sys},S_{\text{out}}}} = \frac{t_{S_{\text{in}}} \times |r_{S_{\text{in}}}|}{T^2_{\text{sys},S_{\text{in}}}} + \frac{t_{\text{obs}} \times |r_{\text{obs}}|}{T^2_{\text{sys,obs}}}$$

$f_{\mathrm{res}}, S_{\mathrm{out}}$

$$(f_{\mathrm{off},S_{\mathrm{out}}} - x_{\mathrm{val},S_{\mathrm{out}}})/f_{\mathrm{res},S_{\mathrm{out}}}$$

$$f(i_{\text{chan}}) = f_{\text{res}} \times (i_{\text{chan}} - r_{\text{chan}}) + f_{\text{off}}$$

$i_{\text{chan}} = 0$

$$x_{\mathrm{val}} = f_{\mathrm{res}} \times (0 - r_{\mathrm{chan}}) + f_{\mathrm{off}}$$

$v_{\mathrm{res}, S_{\mathrm{out}}}$

$$-c \times f_{\mathrm{res},S_{\mathrm{out}}} / f_{\mathrm{rest},S_{\mathrm{out}}}$$

c


$v_{\text{off}}, S_{\text{out}}$


$v_{\text{off}}, S_{\text{in}}$

$$\left(v_{\mathrm{off},S_{\mathrm{out}}} - x_{\mathrm{val},S_{\mathrm{out}}}\right)/v_{\mathrm{res},S_{\mathrm{out}}}$$

$-f_{\mathrm{rest},S_{\mathrm{out}}} \times v_{\mathrm{res},S_{\mathrm{out}}}/c$